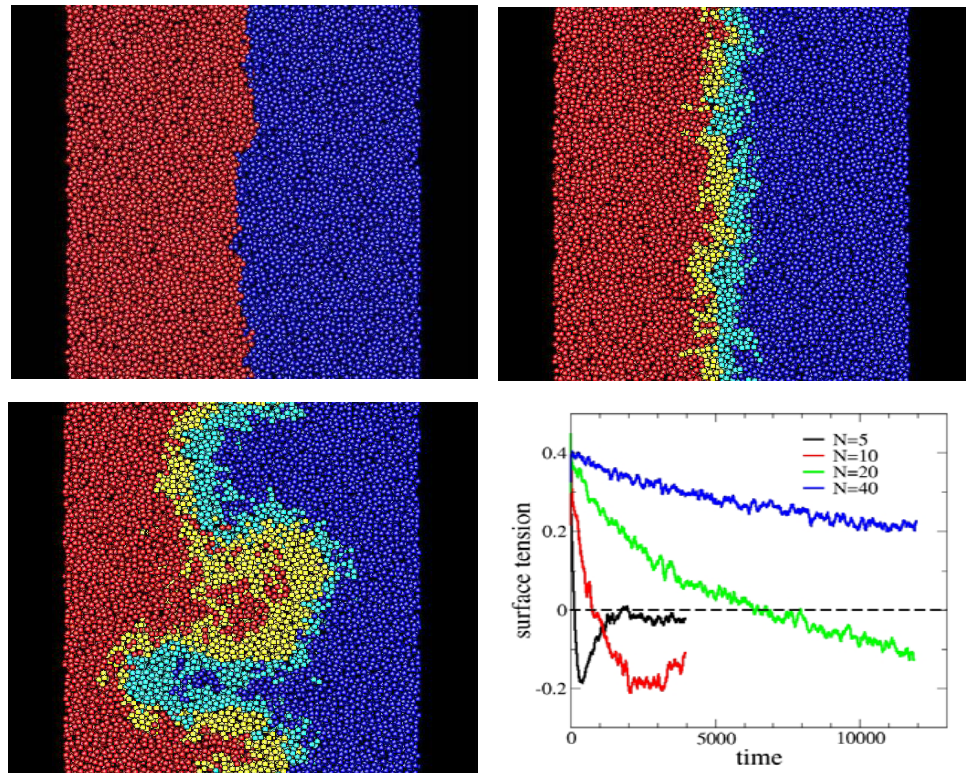


# Modeling of Reactive Compatibilization of Polymer Blends

Chuck Yeung, Pennsylvania State University at Erie, DMR-9986879

Blending two or more polymer species is a cost effective way to produce composites with desirable properties. One way to strengthen adhesion is by adding complementary reactive groups so that the polymers react at the interface to form a copolymer layer. The copolymer layer holds the interface together mechanically and by reducing the surface tension.

Here we present a dissipative molecular dynamics simulation of the formation of the copolymer layer during reactive compatibilization. The polymer interface becomes unstable with increasing copolymer density. The instability is due to the surface tension vanishing.



•C.Yeung and K. Herrmann, *Macromolecules* **36**, 229 (2003).

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## Education:

Three undergraduates (Charles Barr, Kim Herrmann and Andrew Wood) worked or are working on this project. Kim Herrmann is a co-author of our Macromolecules paper and also presented her work at the American Physical Society March Meeting in Indianapolis in 2002 and at the National Conference for Undergraduate Research. She graduated in 2002 with highest honors and is now a graduate student in the Department of Astronomy and Astrophysics at Penn State University where she received an Astronomy Department Fellowship. Charles Barr and Andrew Wood are students at Penn State Erie in physics and computer science respectively.

## Outreach:

The PI participated in the Math Options Program at Penn State Erie. The Math Options Program brings local middle school girls to campus and exposes them to different fields in science and engineering.